Microscopic Foundation and Simulation of Coupled Carrier-Temperature Diffusion Equations in Semiconductor Lasers

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ABSTRACT

A typical semiconductor-based optoelectronic device, such as a diode laser, consists of three subsystems: an optical field, an electron-hole plasma (EHP), and a host crystal lattice. The physics of such a device involves the interplay of optical, electrical and thermal processes. A proper description of such a device requires that all three processes are treated on equal footing and in a self-consistent fashion. Furthermore, since a semiconductor laser has intrinsic spatial inhomogeneity, such a self-consistency naturally leads to a set of partial differential equations in space and time.

There is a significant lacking of research interest and results on the transport aspects of optical devices in the literature with only a few exceptions[1-3]. Even the most important carrier diffusion coefficient has not been properly derived and studied so far for optically excited plasma, while most of the work adopted results from electronics community where heavily doped semiconductors with mainly one type of carriers are dealt with. The corresponding transport equation for plasma energy or temperature has received even less attention. In this talk we describe our recent results [4-6] on such a self-consistent derivation of temperature and carrier-density diffusion equations coupled with the lasing process.

Starting from the microscopic semiconductor Bloch equations (SBEs) including the Boltzmann transport terms in the distribution function equations for electrons and holes, we derived a closed set of diffusion equations for carrier densities and temperatures with self-consistent coupling to Maxwell's equation and to an effective optical polarization equation. The coherent many-body effects are included within the screened Hartree-Fock approximation, while scatterings are treated within the second Born approximation including both the in- and out-scatterings. Microscopic expressions for electron-hole (e-h) and carrier-LO (c-LO) phonon scatterings are directly used to derive the momentum and energy relaxation rates. These rates expressed as functions of temperatures and densities lead to microscopic

expressions for self- and mutual-diffusion coefficients in the coupled density-temperature diffusion equations. Approximations for reducing the general two-component description of the electron-hole plasma (EHP) to a single-component one are discussed. In particular, we show that a special single-component reduction is possible when e-h scattering dominates over c-LO phonon scattering. The ambipolar diffusion approximation is also discussed and we show that the ambipolar diffusion coefficients are independent of e-h scattering, even though the diffusion coefficients of individual components depend sensitively on the e-h scattering rates. Our discussions lead to new perspectives into the roles played in the single-component reduction by the electron-hole correlation in momentum space induced by scatterings and the electron-hole correlation in real space via internal static electrical field. Finally, the theory is completed by coupling the diffusion equations to the lattice temperature equation and to the effective optical polarization which in turn couples to the laser field.

The equations derived above are implemented in various limiting cases to a typical diode laser to study the consequences of nonlinear diffusion and the cross diffusion terms on laser behavior, especially the dynamic behavior of a diode laser under modulation. Detailed results will be presented by comparing with the standard rate equation results.

References

[1] H. Haug and S.W. Koch, Phys. Rev.,**A 39**, 1887(1989).

[2] O. Hess and T. Kuhn, Phys. Rev.,**A 54**, 3347(1996).

[3] J.R. Meyer, Phys. Rev., **B 21**, 1554 (1980).

[4] C.Z. Ning and J.Li, Phys. Rev. B, **65**, 201305(2002).

[5] J.Li and C.Z. Ning, Phys. Rev. A (to appear).

[6] J.Li and C.Z. Ning, Phsy. Rev. A, (to appear).

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OUTLINE

I. Introduction
II. Equations of Motion
III. Moment Equations

II. Equations of Motion:

Density Matrix Equations for Inhomog. Semiconductor (Kuhn, 1994)

- Hamiltonian for a 2-band 2D e-h plasma

$$H = \sum_{k} \left[e_k^e a_k^+ a_k + e_k^h b_{-k}^+ b_{-k} \right] + \frac{1}{2} \sum_{k,k',q\neq 0} V_q \left[a_{k+q}^+ a_{k'-q}^+ a_{k'} a_k + b_{k+q}^+ b_{k'-q}^+ b_{k'} b_k - 2 a_{k+q}^+ b_{k'-q}^+ b_{k'} a_k \right] - \sum_{k} \left[\mu_k a_k^+ b_{-k}^+ + h.c. \right]$$

where $e_k^e = \varepsilon_{g,0} + \frac{\hbar^2 k^2}{2m_e}$, and $e_k^h = \Delta\varepsilon_{CH} + \frac{\hbar^2 k^2}{2m_h}$

- The Heisenberg Equation for the bilinear operator combinations

$$\dot{Q}_{kk'} = \frac{i}{\hbar}\left[H, Q_{kk'}\right]$$

$$Q_{kk'} = a_k^+ a_{k'},\ b_{-k}^+ b_{-k'} \text{ or } b_{-k} a_{k'}$$

Density Matrix Equations (continued)

- Non-diagonal density matrix elements in momentum representation

$$n_{\mathbf{k},\mathbf{k}'}^e = \left\langle a_{\mathbf{k}}^+ a_{\mathbf{k}'} \right\rangle \quad n_{\mathbf{k},\mathbf{k}'}^h = \left\langle b_{\mathbf{k}}^+ b_{\mathbf{k}'} \right\rangle \quad p_{\mathbf{k},\mathbf{k}'} = \left\langle b_{-\mathbf{k}}^+ a_{\mathbf{k}'} \right\rangle$$

- Non-diagonal density matrix elements in "mixed" (Wigner) representation [integro-differential equations, (Kuhn, 1994)]

$$\mathbf{K} = (\mathbf{k} + \mathbf{k}')/2; \quad \mathbf{q} = \mathbf{k} - \mathbf{k}'$$

Fourier transform w.r.t the relative momentum

$$n^\alpha(\mathbf{K}, \mathbf{r}) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} n^\alpha_{\mathbf{K}-\mathbf{q}/2,\mathbf{K}+\mathbf{q}/2} \qquad (\alpha = e, h)$$

$$p(\mathbf{K}, \mathbf{r}) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} p_{\mathbf{K}-\mathbf{q}/2,\mathbf{K}+\mathbf{q}/2}$$

Density Matrix Equations (continued)

- Taylor expansion of the density matrices:

$$f_{\mathbf{K}-\mathbf{k}}(\mathbf{R}-\mathbf{r}) = \sum_{n,m=0}^{\infty} \frac{1}{n!\,m!}\left(-\mathbf{r}\bullet\frac{\partial}{\partial \mathbf{R}}\right)^{n}\left(-\mathbf{k}\bullet\frac{\partial}{\partial \mathbf{K}}\right)^{m} f_{\mathbf{K}}(\mathbf{R})$$

with

$$(-\mathbf{r})^{n} e^{i\mathbf{k}\bullet\mathbf{r}} = i^{n}\frac{\partial^{n}}{\partial \mathbf{k}^{n}} e^{i\mathbf{k}\bullet\mathbf{r}} \qquad (-\mathbf{k})^{m} e^{\pm i\mathbf{k}\bullet\mathbf{r}} = (\pm i)^{m}\frac{\partial^{m}}{\partial \mathbf{r}^{m}} e^{\pm i\mathbf{k}\bullet\mathbf{r}}$$

- Final equations of motion
  - To first order of Taylor expansion
  - Ignore explicit spatial variation of polarization variables

Maxwell-Bloch-Boltzmann-Poisson Eqns.

$$\frac{1}{c^{2}}\partial_t^2 E - \nabla_{\mathbf{R}}^2 E = -\frac{1}{\varepsilon_0 c^2}\partial_t^2(\wp_a + \wp_b)$$

$$\partial_t n^{\alpha} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon^{\alpha}\bullet\nabla_{r} n^{\alpha} - \frac{1}{\hbar}\nabla_{r}\left[\delta\varepsilon^{\alpha} + q^{\alpha}\Phi\right]\bullet\nabla_{\mathbf{k}} n^{\alpha} = R^{\alpha} + \partial_t n^{\alpha}\big|_{col.}$$

$$\partial_t p = -\frac{i}{\hbar}\left[\varepsilon^{e} + \varepsilon^{h}\right]p - i\Omega\left[n^{e} + n^{h} - 1\right] + \partial_t p^{\alpha}\big|_{col.}$$

$$\nabla_r^2 \Phi = -\frac{1}{\varepsilon_0\varepsilon_b}\frac{2}{V}\sum_{\alpha,\mathbf{k}} q^{\alpha} n^{\alpha}$$

(Hess and Kuhn, 1996)

$n^{\alpha} = n^{\alpha}(\mathbf{k}, r)$: distributi on functions $(\alpha = e, h)$

$p = p(\mathbf{k}, r)$: interband polarizati on

$E = E(\mathbf{R}, t)$: optical field; $\wp_b$: background polarizati on

$\wp_a = \frac{2}{V}\sum_{\mathbf{k}}\left[\mu^{*} p(\mathbf{k}, r) + c.c\right]$: active medium polarizati on

Definitions and Expressions in MBBP Equations

$$R^{\alpha} = \Lambda^{\alpha} - R_{sp}^{\alpha} + i\left[\Omega(\mathbf{k},\mathbf{r})p^{*}(\mathbf{k},\mathbf{r}) + c.c\right]$$

$$\varepsilon^{\alpha} = \varepsilon_{0}^{\alpha}(\mathbf{k}) + q^{\alpha}\Phi + \delta\varepsilon^{\alpha}(\mathbf{k},\mathbf{r})$$

$\delta\varepsilon^{\alpha}(\mathbf{k},\mathbf{r}) =$ [redacted]

$\hbar\Omega = \mu(\mathbf{k})E(\mathbf{r},t) +$ [redacted]

$\partial_t n^{\alpha}\big|_{col.} =$ [redacted] $+ \partial_t n^{\alpha}\big|_{LO}$

$\partial_t p^{\alpha}\big|_{col.} =$ [redacted]

Γ_{out}, Γ_{in} real

Bandgap renormalization due to scatterings taken into account using screened potential

Carrier-Carrier and Carrier-LO Phonon Scattering Terms in SBEs

$$\Gamma_{out}(\mathbf{k}) = \sum_{\alpha,\beta,\mathbf{k},\mathbf{k}',\mathbf{q}\neq 0} C_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\alpha\beta}\left\{n_{\mathbf{k}+\mathbf{q}}^{\alpha} n_{\mathbf{k}'}^{\beta}\left(1 - n_{\mathbf{k}'+\mathbf{q}}^{\beta}\right) + n_{\mathbf{k}'+\mathbf{q}}^{\beta}\left(1 - n_{\mathbf{k}'}^{\beta}\right)\left(1 - n_{\mathbf{k}+\mathbf{q}}^{\alpha}\right)\right\}$$

$$\Gamma_{in}(\mathbf{k},\mathbf{k}') = \sum_{\alpha,\beta,\mathbf{k},\mathbf{q}\neq 0} C_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\alpha\beta}\left\{n_{\mathbf{k}}^{\alpha} n_{\mathbf{k}'+\mathbf{q}}^{\beta}\left(1 - n_{\mathbf{k}'}^{\beta}\right) + n_{\mathbf{k}'}^{\beta}\left(1 - n_{\mathbf{k}'+\mathbf{q}}^{\beta}\right)\left(1 - n_{\mathbf{k}}^{\alpha}\right)\right\}$$

$$\partial_t n_{\mathbf{k}}^{\alpha}\big|_{e-h} = \sum_{\mathbf{k}',\mathbf{q}\neq 0} C_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\alpha\beta}\left\{n_{\mathbf{k}+\mathbf{q}}^{\alpha} n_{\mathbf{k}'}^{\beta}\left(1 - n_{\mathbf{k}'+\mathbf{q}}^{\beta}\right)\left(1 - n_{\mathbf{k}}^{\alpha}\right) + n_{\mathbf{k}}^{\alpha} n_{\mathbf{k}'+\mathbf{q}}^{\beta}\left(1 - n_{\mathbf{k}'}^{\beta}\right)\left(1 - n_{\mathbf{k}+\mathbf{q}}^{\alpha}\right)\right\}$$

$$\partial_t n_{\mathbf{k}}^{\alpha}\big|_{LO} = -\sum_{\mathbf{q}}\left[W_{\mathbf{k}-\mathbf{q},\mathbf{k}}^{\alpha} n_{\mathbf{k}}^{\alpha}\left(1 - n_{\mathbf{k}-\mathbf{q}}^{\alpha}\right) - W_{\mathbf{k},\mathbf{k}-\mathbf{q}}^{\alpha} n_{\mathbf{k}-\mathbf{q}}^{\alpha}\left(1 - n_{\mathbf{k}}^{\alpha}\right)\right]$$

where $C_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\alpha\beta} = \frac{2\pi}{\hbar} V_{s,\mathbf{q}}^{2}\,\delta\left(\varepsilon_{\mathbf{k}}^{\alpha} + \varepsilon_{\mathbf{k}'+\mathbf{q}}^{\beta} - \varepsilon_{\mathbf{k}'}^{\beta} - \varepsilon_{\mathbf{k}+\mathbf{q}}^{\alpha}\right)$

$$W_{\mathbf{k}-\mathbf{q},\mathbf{k}}^{\alpha} = \frac{2\pi}{\hbar}\sum_{z}\left|\gamma_{\mathbf{q}}^{\alpha}\right|^{2}\delta\left(\varepsilon_{\mathbf{k}-\mathbf{q}}^{\alpha} - \varepsilon_{\mathbf{k}}^{\alpha} \pm \hbar\omega_{LO}\right)\left(N_{Q} + \frac{1}{2} \pm \frac{1}{2}\right)$$

Features of Our Approach

- Coherent part contains both exchange interaction and [redacted] term in the bandgap renormalization
- Full microscopic second order scattering terms treated without assuming [redacted] in the Boltzmann equation

$$\cancel{\partial_t n^\alpha\big|_{col} = -\frac{1}{\tau}\left[n^\alpha - f^\alpha\right]}$$

  - Cancellation of e-h scattering terms for ambipolar diffusion coefficients
  - Detailed expression for all diffusion coefficients in terms of distribution functions

III. Moment Equations (Hydrodynamic Equations)

- Moment $\mathbf{M}_n^\alpha$ and current $\mathbf{J}_n^\alpha$ of nth order:

$$\mathbf{M}_n^\alpha(\mathbf{r}) = \frac{2}{S}\sum_{\mathbf{k}} \mathbf{F}_n^\alpha n^\alpha(\mathbf{r}), \quad \mathbf{J}_n^\alpha(\mathbf{r}) = \frac{2}{S}\sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}}^\alpha \mathbf{F}_n^\alpha n^\alpha(\mathbf{r})$$

with $\mathbf{F}_n^\alpha = 1, \hbar\mathbf{k}, \frac{\hbar^2\mathbf{k}^2}{2m_\alpha}$ for $n = 0, 1, \text{and } 2$

- Derivation of moment equations

$$\partial_t \mathbf{M}_n^\alpha(\mathbf{r}) = \frac{2}{S}\sum_{\mathbf{k}} \mathbf{F}_n^\alpha \partial_t n^\alpha(\mathbf{r})$$

Or apply operator $\frac{2}{S}\sum_{\mathbf{k}} \mathbf{F}_n^\alpha(\bullet\bullet\bullet)$ on both sides of Boltzmann equation

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- The "hierarchy" problem
  - Order-n currents are related to order-(n+1) moments
  - Existence of polarization variable $p(\mathbf{k},\mathbf{r})$ leads to terms such as

$$\frac{2}{S}\sum_{\mathbf{k}} \mathbf{F}_n^\alpha p(\mathbf{k},\mathbf{r}), \text{ and } \frac{2}{S}\sum_{\mathbf{k},\mathbf{k}'} \mathbf{F}_n^\alpha p(\mathbf{k},\mathbf{r}) V_{s,\mathbf{k}-\mathbf{k}'} p(\mathbf{k}',\mathbf{r})$$

- Cutting-off the hierarchy
  - Isotropy or ignoring non-diagonal tensor components of 2nd moment
  - Quasi-equilibrium with a non-zero-drift momentum $\mathbf{k}_D^\alpha$

$$n^\alpha(\mathbf{k},\mathbf{r}) = f^\alpha_{\mathbf{k}-\mathbf{k}_D^\alpha} = \left\{1 + \exp\left[\frac{\varepsilon^\alpha_{\mathbf{k}-\mathbf{k}_D^\alpha} - \mu_F^\alpha(\mathbf{r})}{k_B T^\alpha(r)}\right]\right\}^{-1}$$

- Moment-current relations up to 2nd order

$$\left(\mathbf{M}_0^\alpha, \mathbf{M}_1^\alpha, \mathbf{M}_2^\alpha\right) \equiv \left(N^\alpha, \mathbf{P}^\alpha, E^\alpha\right) \qquad \left(\mathbf{J}_0^\alpha, \mathbf{J}_1^\alpha, \mathbf{J}_2^\alpha\right) \equiv \left(\mathbf{J}_N^\alpha, \mathbf{J}_P^\alpha, \mathbf{J}_E^\alpha\right)$$

[redacted]

$$\mathbf{P}^\alpha = m_\alpha \mathbf{u}^\alpha N^\alpha = \hbar\mathbf{k}_D N^\alpha \qquad E^\alpha = W^\alpha + E_D^\alpha$$

$$W^\alpha \equiv \frac{2}{S}\sum_{k} \frac{\hbar^2 k^2}{2m_\alpha} f_{\mathbf{k}}^\alpha \qquad E_D^\alpha = \frac{1}{2} m_\alpha \left|u^\alpha\right|^2 N^\alpha$$

- Linearizing scattering terms $\partial_t \mathbf{M}_n^\alpha(\mathbf{r})\big|_{col} \equiv \frac{2}{S}\sum_{\mathbf{k}} \mathbf{F}_n^\alpha \partial_t n^\alpha(\mathbf{r})\big|_{col}$

The Hydrodynamic Equations

$$\partial_t N^\alpha + \nabla_{\mathbf{r}} \bullet \left(\mathbf{u}^\alpha N^\alpha\right) = R_N^\alpha \qquad (\alpha \neq \beta = e,h)$$

$$\partial_t \mathbf{P}^\alpha + \nabla_{\mathbf{r}} \bullet \left(\mathbf{u}^\alpha \mathbf{P}^\alpha\right) + \nabla_{\mathbf{r}} W^\alpha + N^\alpha \nabla_{\mathbf{r}} \left(\text{[redacted]} + q^\alpha \Phi\right)$$
$$= R_{\mathbf{P}}^\alpha - \text{[redacted]} \mathbf{P}^\alpha + \text{[redacted]} \mathbf{P}^\beta - \gamma_{LO}^\alpha \mathbf{P}^\alpha$$

$$\partial_t W^\alpha + \nabla_{\mathbf{r}} \bullet \left(2\mathbf{u}^\alpha W^\alpha\right) - \mathbf{u}^\alpha \bullet \nabla_{\mathbf{r}} W^\alpha$$
$$= R_W^\alpha - \text{[redacted]} \left(T^\alpha - T^\beta\right) - \Gamma_{LO}^\alpha \left(T^\alpha - T_{LO}\right)$$

- Explicit, closed form hydrodynamic equations derived microscopically for e-h system
- Describe e-h dynamics in optically-excited semiconductors such as in THz generations, photoconductive switches, and lateral photodetectors

* Effects of Lateral Diffusion under constant injection

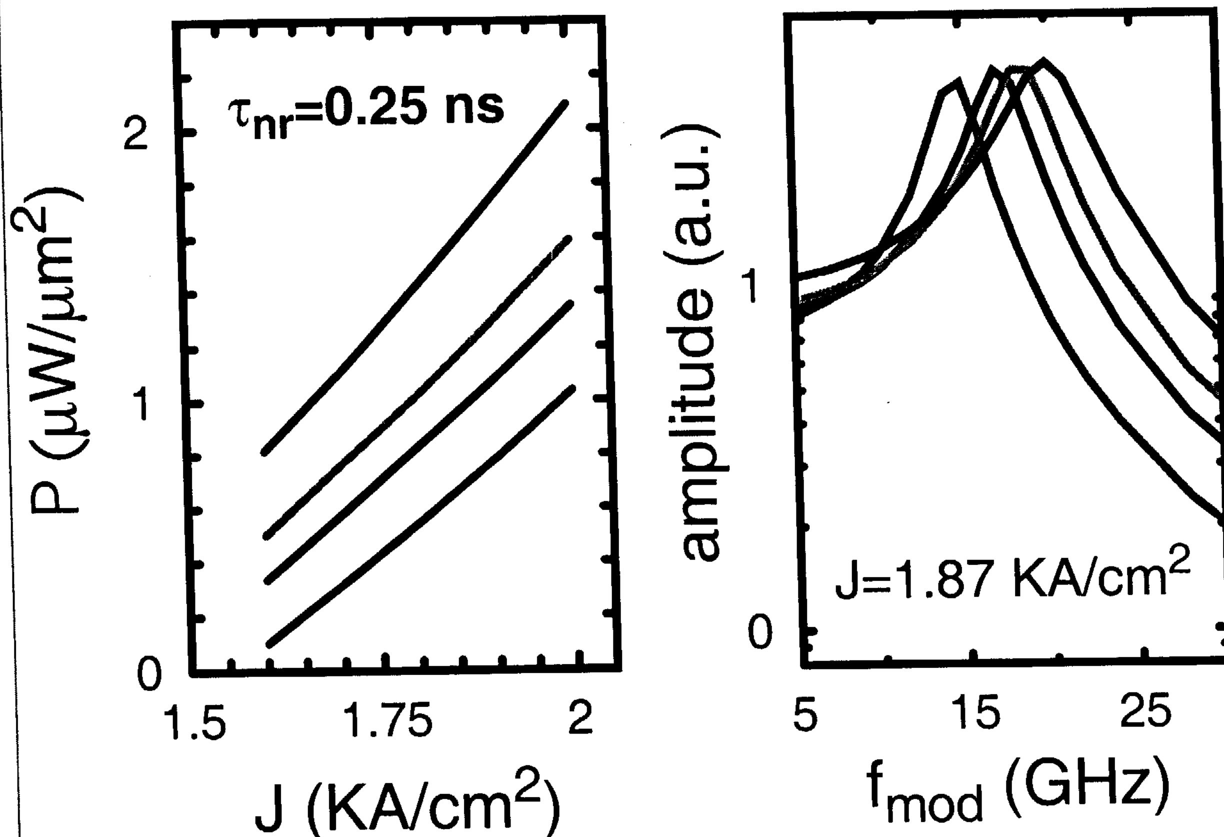
(F): $D_{NN}(N)$
Nonlinear

(a): 2.5×10^{12} cm^{-2},
54.115 cm^2/s

(b): 7×10^{11} cm^{-2},
23.838 cm^2/s

(c): 2.5×10^{10} cm^{-2},
7.5 cm^2/s

DC: $P=\alpha(J-J_{th})$ AC: responsivity



* DC and AC Effects of Lateral Diffusion

(2) AC effects